Institute for Scientific Computing Research

University Collaborative Research Program Proposals

Center for Applied Scientific Computing

Software Infrastructure for Multi-Tier Implementation of Structured Adaptive Mesh Hierarchies

Scott Baden

University of California, San Diego

Abstract

The Principal Investigator (PI) proposes to investigate and develop a scalable portable programming methodology and software tool for efficiently implementing structured adaptive mesh refinement on multi-tier computers, which are multi-computers comprising symmetric multiprocessor (SMP) nodes. The program will leverage the investigator's previous work with the KeLP system. This C++ class library provides hierarchical SMPD control flow to manage two levels of parallelism and locality.[1] The primary research issue addressed by the investigation is to develop a "communication aware" multi-tier load-balancing strategy that includes communication as part of the computational workload, and permits the application programmer to mask the latency and overhead of communication.

This research builds on the PI's previous experience with structured adaptive elliptic solvers running on MPPs.[2] The investigation will deliver a computational testbed permitting Lawrence Livermore National Laboratory scientists to explore portable, scalable implementations of adaptive mesh applications running on a variety of platforms of interest to the Laboratory. This investigation is timely, as it will provide a practical technique for effectively utilizing not only cluster of SMPs, but also high-end ASCI platforms such as the IBM ASCI Blue–Pacific machine. Current approaches based on employing MPI alone are not scalable. The PI will collaborate with Jonathan May (CASC) to carry out performance analysis of the software infrastructure and to establish contact with potential laboratory users.

[1] KeLP is part of the thesis research of Ph.D. student Stephen J. Fink, who is funded by a DOE Computational Graduate Student Fellowship.

[2] This pre-existing collaboration involves Scott Kohn (CASC), Beth Ong (CASC), and John Weare (UCSD, Chemistry).

Computational Fluid Dynamic Studies of Arterial Flow Disturbance Induced by Intravascular Stents

Abdul Barakat

University of California, Davis

Abstract

Atherosclerosis is an arterial disease whose pathological complications, namely heart disease and stroke, are the leading cause of mortality in the industrialized world. In its advanced form, atherosclerosis leads to plaques that protrude into arterial lumens and form stenosis or even complete vessel occlusions, which obstruct blood flow and give rise to the pathological events. One common interventional procedure involves the placement of an intravascular stent, an expandable wire mesh structure, that is introduced into the diseased artery in a compressed state and is inflated at the stenosis or occlusion site to both restore blood flow and provide structural stability to the arterial wall. The major limitation to the success of this procedure, however, is restenosis, a complex and incompletely understood process by which plaques re-protrude into the vessel lumen within a period of a few months.

The placement of a stent in an artery mechanically damages the endothelium, the monolayer of cells lining the inner surface of all blood vessels. In vitro data indicate that the rate of endothelial repair after injury may be significantly slower in regions in which endothelial cells are exposed to relatively large fluid mechanical shear stress gradients, as occurs at the end points of flow separation zones. Therefore, flow separation in the vicinity of a stent may contribute to restenosis. The hypothesis driving our research is that the occurrence of flow separation depends on appropriate hemodynamic matching between the stent design and the flow and geometric properties of the arterial segment in which the stent is positioned. We propose to test this hypothesis by studying the impact of various geometric and flow parameters on the occurrence of near-stent flow separation using computational fluid dynamic techniques. We shall use the spectral-element fluid dynamic code NEKTON to accomplish this goal. Our specific aims are

- To perform three-dimensional steady-flow simulations of the flow simulations of the flow field in the vicinity of an intravascular stent positioned within a straight rigid-wall arterial segment.
- To extend the simulations to physiological pulsatile flow.
- To perform three-dimensional steady and pulsatile flow simulations of the flow field in the vicinity of an intravascular stent positioned within a curved arterial segment.
- To incorporate certain aspects of arterial wall motion into the simulations.

The proposed collaboration with LLNL is critical to the successful completion of the research for two principal reasons

- LLNL's supercomputer capabilities will be needed for the solution of the equations in the some of the more computationally intensive simulations.
- Hydrodynamic simulation capabilities currently under development at LLNL may, in the future, allow the incorporation of additional physiological considerations into the aortic model including fluid-wall coupling. Furthermore, results of the proposed research will define possible future collaborations with the Center for Health Care Technologies at Lawrence Livermore National Laboratory. Of particular interest are the areas of actuation mechanisms for the deployment of miniature devices within blood vessels, and the application of imaging modalities to better characterize the effect of stent placement on the arterial wall.

Parallel Multigrid Methods on Unstructured Grids for Scientific Computing

Tony Chan

University of California, Los Angeles

Abstract

We propose to investigate efficient multigrid methods for elliptic problems on unstructured grids that are suitable for distributed and shared memory parallel computing architectures. Two aspects of multigrid will be studied in this work.

The first is the design of optimized multigrid libraries for elliptic problems that are robust with respect to the mesh size and the coefficient of the PDEs. The second is the performance of various multigrid algorithms on parallel computers. Particular emphasis will be placed on multigrid algorithms appropriate for solving the discretization matrices arising from various large-scale scientific computing problems such as plasma physics simulations, turbulence flow, ground water flow, and the like.

University of California
Lawrence Livermore National Laboratory

Renewal of a Collaborative UCLA–LLNL Program on Parallel PIC Modeling of Semiclassical Quantum Models

Viktor Decyk
and
John Dawson

University of California, Los Angeles

Abstract

We propose to continue a collaborative program between University of California Los Angeles and Lawrence Livermore National Laboratory on parallel computing applied to particle-in-cell (PIC) codes. We have been successful in modeling many particle quantum systems by combining a semiclassical approximation of Feynman path integrals with parallel computing techniques previously developed at UCLA for simulating plasmas. With continued support, we should be able to construct a complete multiparticle quantum mechanical modeler.

Massively Parallel Computations Applied to Finite Element Analysis

Tony Keaveny

University of California, Berkeley

Abstract

Detailed stress analysis of trabecular bone, which has a highly complex and heterogeneous microstructure and unknown tissue properties, will improve understanding of its mechanical behavior, and accelerate progress in a number of biological and medical studies. Our goal in this continuing study is to utilize a unique finite element analysis method to study the failure behavior of trabecular tissue. Typically, these finite element models have 1–100 million elements and cannot be analyzed in an efficient manner using conventional finite element techniques.

During the first two years of this grant, a custom finite element code was developed which allows large models with more than one million elements to be efficiently solved using parallel computational techniques. Our code was used to study the convergence behavior of the models, and later to predict the elastic properties of trabecular tissue. The current proposal is to continue refining this analysis method and to then use it to study the failure behavior of trabecular tissue. As with our previous work on elastic behavior of trabecular bone, using this analysis technique, our proposed studies will combine extensive mechanical testing data available from ongoing experiments at UC Berkley with results from the finite element analyses to ensure model validation. This work will be beneficial to Lawrence Livermore National Laboratory, as it will establish computational techniques that can be used for a variety of future research in computational biomechanics. These research areas include the effects of aging, bone injury, and osteoporosis.

Development of a Three-Dimensional Relativistic Particle-In-Cell Code for Studying the Production of Useful Electron Bunches Using Ultra-Intense Laser Pulses

Warren Mori

University of California, Los Angeles

Abstract

This is a continuation proposal for the "development of a parallelized three-dimensional (3D) relativistic particle-in-cell (PIC) code for studying the production of useful electron bunches using ultra-intense laser-pulses."

During the past year, we developed an object-oriented skeleton code for 3D parallel PIC algorithms, studied laser-wakefield excitation in 3D using a code with the local charge conserving algorithm of Marder (Langdon's improvement), and studied the electron beam characteristics for laser-driven wavebreaking and optical injection techniques in 2D. We propose to incorporate the 2D and 3D algorithms into the object oriented skeleton code, to benchmark these and other algorithms, and to investigate the production of useful electron bunches in 3D and 2D.

A Computational Investigation of Finite-Strain Plasticity Model for Crystalline Solids

Panayiotis Papadopoulos

University of California, Berkeley

Abstract

The proposed investigation is a continuation of current research on the development of a Lagrangian finite element-based computational framework for the analysis of initial/boundary-value problems of macroscopic rate-independent elastoplasticity, based on the theory of Green and Naghdi. The proposed work will concentrate on incorporating microstructural effects into the computational formulation, with particular emphasis on single crystals and polycrystalline aggregates. Detailed constitutive models within the above theoretical framework will be formulated and numerically analyzed in collaboration with ongoing research at Lawrence Livermore National Laboratory. This research focuses on experimental measurements in finitely deforming polycrystalline solids.

Method of Simulation for Localized Multiply-Scaled Condensed Materials

John Weare

University of California, San Diego

Abstract

Many materials of technological importance are of mixed composition, lack symmetry, and display complex chemical bonding patterns. All of these factors complicate the prediction of their structural properties. To make matters worse, the simulation of physical properties of such materials often requires dynamic information (e.g., prediction of reactivity or high-temperature pressure behavior). Typically, bonding interactions between particles for these materials are strong and many-body. This means that equations of motion must be solved in detail to predict dynamics. Since atomic particles are massive, the dynamics can be simulated directly using Newton's laws, as in molecular dynamics (MD). However, materials with covalent, metallic, and even hydrogen bonding are difficult to describe succinctly with simple analytical inter-particle potentials, making them difficult to simulate with traditional MD approaches.

Recently, considerable progress has been made with the introduction of *ab-initio* molecular dynamics (AIMD) methods. These method are similar in intent to traditional MD simulation methods, except that the forces necessary to propagate the system are calculated from very fast solutions of the electronic Schrodinger equation within the Local Density Approximation (LDA). This greatly generalizes the application of MD and has made possible considerable progress in material simulation. However, there are still very significant limitations to the application of these approaches, particularly for systems with highly bound electrons such as O, F, and the transition metals.

The research program proposed here is designed to both develop new methods of simulations targeted at these difficult elements and make progress in the actual simulation of materials of direct interest to research programs at Lawrence Livermore National Laboratory (LLNL). The progress in simulation will come from the more efficient parallel implementation of existing methods and from the development of new simulation approaches. The proposed methods will more efficiently resolve the electronic wavefunctions in regions of rapid variation and, thereby, focus computer memory and CPU cycles in the portions of the computational domain where they are most needed.

We will pursue two methods. The first represents a continuation of our previous efforts to implement a structured adaptive finite element method that places structured grids of increasing refinement in regions requiring higher resolution (e.g., near atom centers). We have already made some progress with this approach; however, we have found that we need to go to more accurate discretizations to obtain the required chemical accuracy. We are hoping that chemically accurate results can be obtained by a local application of spectral element methods. The second approach to local enhancement is to use a mixed basis set of planewaves augmented by a linear local basis confined to regions near the atomic centers. This would amount to a dynamic implementation of LAPW methods. LAPW methods are known to perform well for these systems. However, it will be a challenge to develop a parallel algorithm efficient enough to allow dynamics for sufficiently long simulation periods.

One objective of LLNL's H Division is the development of simulation methods capable of predicting high-temperature high-pressure behavior in the system $HF - CO_2 - CH_4\ H_20 - N_2$. For the temperatures and pressures of interest (T≈3400 K and P≈32 GPa), there is very little data available, even for the pure end members. This is particularly true of the HF system because of its corrosive nature. The intention of this program is to replace unavailable experimental data by computational data for moderately sized systems. The presence of O, N, and F make this a difficult problem for AIMD. However, preliminary calculations have shown that HF can be

calculated with high accuracy by choosing a softened pseudopotential. Since the number of valence electrons in each of these molecules is relatively small, we expect that we will be able to simulate systems of the order of 40 molecules with our present algorithm. This will require fast implementations of our codes on LLNL's parallel supercomputers, and the efficient utilization of memory hierarchy. We believe that the present solver algorithms can also be improved by preconditioning the conjugate gradient iterative method. Furthermore, because the intermolecular interactions in this system are relatively weak (hydrogen bonds), we will need to implement and test density correction approximations. All of this can be accomplished in the first year of the grant.

As we make progress with the new methods, we will use $HF - CO_2 - CH_4 - H_20 - N_2$ as a test of efficiency and accuracy. The proposed computation approaches may be implemented so as to eliminate the requirement of pseudopotentials. All-electron calculations of this sort may be required to treat very high-pressure systems. We emphasize that while the methods the we are developing as part of this grant will be used the treat problems in the $HF - CO_2 - CH_4 - H_20 - N_2$ systems, these new methods will also have general application to other problems that involve difficult elements, such as transition elements.